Simulations of Microstructures With Different Degrees of Spatial Clustering Using the Features of Complex Morphologies From Corresponding Real Microstructure

PI: Arun M. Gokhale

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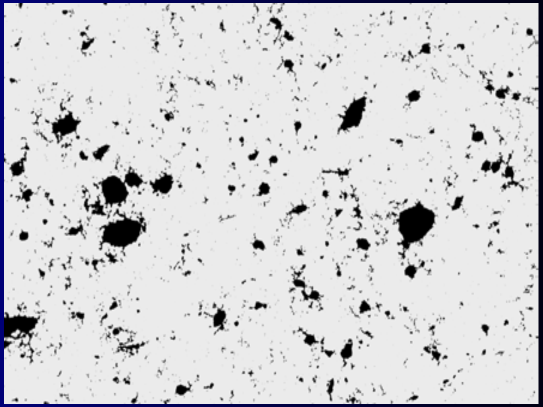
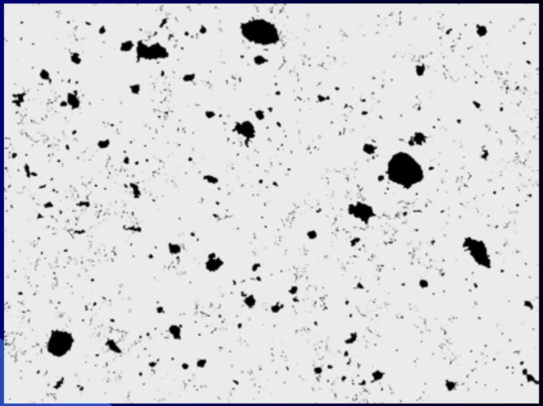
- Spatial arrangement (clustering, etc) of voids, inclusions, etc in microstructure influences properties of materials.
- To deconvolute and quantify the effects of spatial clustering on the properties, it is essential to produce a set of microstructures having different degrees of spatial clustering without varying any other attributes (morphologies, shapes, size distribution, etc.), which is extremely difficult in practice, because the process parameters that affect clustering may also change feature morphologies, sizes, etc.
- Solution: Image analysis procedure to "pluck" out features from a real microstructure, put them in a "box", simulate a spatial arrangement of centroids with known degree of clustering (or repulsion), and place the features from the "box" one by one at simulated centroids to create simulated microstructure with different degrees of clustering that have the same "realistic" particle/void morphologies, and size/shape distribution, volume fraction, etc.
- Example: (a) real microstructure of voids in a cast Mg-alloy) (b) simulated random microstructure having the same images of voids, (c) simulated clustered microstructure having the same voids. These simulations can be implements in the finite elements (FE) computations to deconvolute effects of spatial clustering on micro-mechanical response, void growth, coalescence, etc.


a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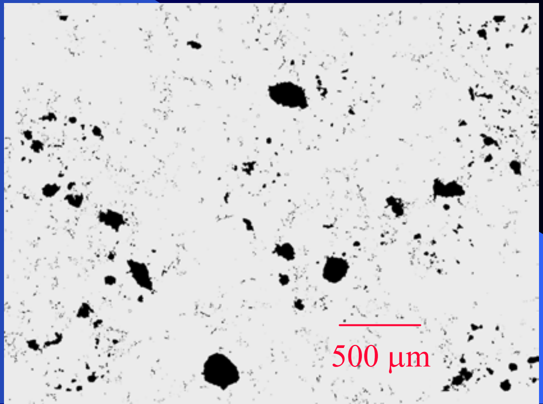
c

Geometric Constraints on N-Point Correlation Functions

PI: Arun M. Gokhale

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• N-point correlation functions are integral part of microstructure representation methodologies and theories. Therefore, modeling of n-point correlation functions is of interest

• It is important to determine if a given mathematical model for n-point correlation function can represent a <u>**physically realizable microstructure**</u>

• A set of geometric constraints have been derived for two-, three-,and four-point correlation functions based on stereological principles, which any physically realizable modeled equation for correlation function must satisfy. The box on the right describes one such constraint of three-point correlation function

• Three-point correlation function P_{112} $(r, \alpha_1, \alpha_2, \theta, \varphi)$ is the probability that a randomly *located* triangle, in a plane of orientation (θ, φ), having base length r and angles α_1 and α_2 is such that the two corners of the triangle that are associated with the base are in the phase-1 (say particles) and the third corner in the phase-2 (matrix).

<u>**Constraint**</u>

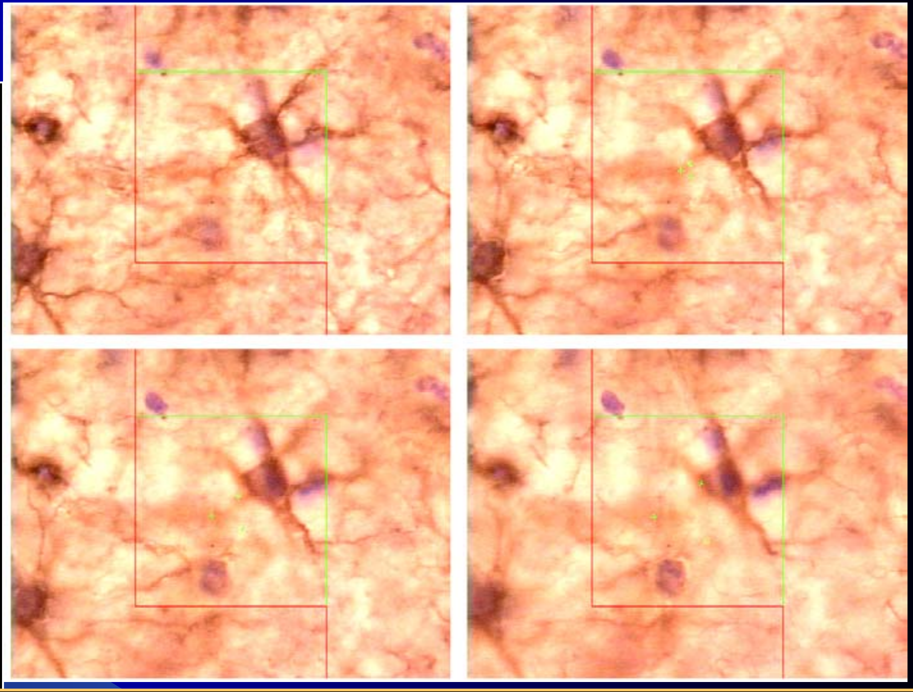
$$\lim \left[P_{112}(r, \alpha_1, \alpha_2\ \theta, \varphi) / \Delta\right] = Q_V/(6\pi)$$

$$r, \alpha_1, \text{and } \alpha_2 \to 0$$

Q_V is the integral <u>absolute</u> mean curvature of the interfaces between the two phases and Δ is the area of the triangle

Similar constraints have been derived for two- and four-point functions

Applications in Other Disciplines: Characterization of Biological Structures
PI: Arun M. Gokhale Award: DMR-9816618/0404668



Study of microstructures is central to numerous disciplines where microscopes are used to characterize internal structures. Stereological techniques for quantitative microstructure characterization are becoming increasingly important in all such disciplines due to the thrust towards quantitative description and modeling of the processes and phenomena of interest. Stereological techniques developed in the NSF funded research have also been applied to quantify internal structures in biological tissues

1. Gokhale, Evans, Mackes, and Mouton: *Unbiased Estimation of Surface Area in Biological Tissue Sections of Arbitrary Orientations Using Virtual Cycloids*, **J. of Microscopy**, in press.

Above: Traverse of virtual cycloids (light green dots) through different focal planes of thick tissue section of DG in mouse brain

The estimated value of the total surface area of the GFAP immunopositive astrocytes per unit vol. of the tissue section = 0.039 $\mu m^2/\mu m^3$

V_{ref} for the DG in mouse brain = 1.9 mm^3

Total surface area of GFAP immunopositive astrocytes = 74.1 mm^2